Title

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Multilayer-coated blazed grating with variable line spacing and a variable blaze angle

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The blazing ability of multilayer-coated blazed gratings (MBG) was systematically investigated via numerical calculation of the diffraction efficiency with a rigorous electromagnetic simulation code. It was found that the blazing condition is not exact and allows significant deviation from the ideal situation for ultra-dense MBGs. A mismatch of the interfaces of the multilayer (ML) stacks of adjacent grooves results in a modified effective blaze angle, which gives the opportunity to control and tune precisely the blaze angle via a proper choice of ML d-spacing. Also this allows a new kind of x-ray gratings which have a variable line spacing (VLS) as well as a variable blaze angle. Precise adjustment of a local blaze angle of a VLS MBG can be achieved with a laterally graded ML, providing very high diffraction efficiency for the whole area of the grating.

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Recent progress in the technology of multilayer-coated blazed gratings (MBG) [1-3] opens important opportunities for the development of a new generation of spectrometers for EUV and soft x-rays [4,5]. The gratings have superior efficiency characteristics over lamellar gratings due to their blazing ability, which is provided by the slanted facets of the saw-tooth grooves. MBGs take advantage of the high reflectance of a multilayer coating under the Bragg condition. To achieve maximum blazing ability, a certain relation between the grating period, $d_{grating}$, blaze angle, ϕ, and multilayer d-spacing, D_{ML}, is required. The optimal ratio for the grating parameters was formulated by Rife et al. [6] as:

$$\frac{d_{grating}\sin\phi}{D_{ML}} = m \qquad (1)$$

where m is an integer number. According to formula (1) the ML d-spacing should be equal to the length of an anti-blazed facet, $h = d_{grating}\sin\phi$, of a saw-tooth groove for blazing into the 1st diffraction order. (Anti-blazed facets are supposed to be perpendicular to the blazed ones for a saw-tooth substrate). For the mth order diffraction order, the length of the anti-blazed facets should be m-fold time the multilayer d-spacing. For example, the "depth" of the grooves should be equal to the doubled ML d-spacing for the 2nd order blazing, or tripled d-spacing for the 3rd order blazing etc. In all the cases the respective layers of neighboring grooves should stitch to each other perfectly without a discontinuity.

There are however a few issues regarding this simple rule. It is not clear how strict the condition given by equation (1) is, i.e. how fast the efficiency decays with deviation from the ideal blazing condition. Our experimental experience in MBG fabrication [1-3] indicates that a modest deviation from (1) is not harmful and in many cases can be tolerated. Another question raised by Underwood et al., [7] is how refraction of x-rays in multilayer media affects the blazing condition. The authors suggested to incorporate an additional term into the equation (1) to take refraction into account. This, however, has never been investigated theoretically or experimentally.

Most modern synchrotron beamline spectrometers and monochromators utilize variable line spacing (VLS) gratings rather than constant groove density gratings due to the fact that flat field focusing and aberration control can all be combined in one element. Their use is particularly critical in applications where very high spectral resolution is required. However, it is not obvious if multilayer coated VLS gratings are possible for these applications. If a VLS substrate is coated with a multilayer with a certain d-spacing, condition (1) will be satisfied only for the center of the grating and with significant deviations for the edges of the grating. Typically the grating pitch for a VLS grating varies up to +/- 20% over the grating length. This means that the right part of the equation (1) will deviate from an integer number significantly, typically in the range of 0.8-1.2 over the grating area. Moreover, the angles of incidence and diffraction are quite different for different parts of a VLS grating. This leads to violation of the Bragg condition for the multilayer and can result in significant efficiency losses. How to circumvent these issues has not been clear and require thorough theoretical and experimental investigation.

In this paper we systematically investigate the dependence of the blazing ability of MBGs on the h/D_{ML} ratio using a commercial code that allows solution of Maxwell's equations in 3d for grating like structures (PCGrate-6.1) [8]. We will show that the blazing condition is actually rather soft, i.e. diffraction efficiency remains quite high even for a significant deviation of the h/D_{ML} ratio from an integer number. This opens the possibility to control the effective blaze angle with a proper choice of the ML d-spacing, and allows a new class of x-ray diffraction grating which are

VLS multilayer-coated blazed gratings (VLS MBG) with a variable blaze angle (VBA).

A sketch of an ideal MBG designed according to the blazed condition (1) is shown in Fig. 1. Layers of high-Z (grey) and low-Z (white) materials are deposited on a saw-tooth substrate (black). Layers of adjacent grooves are perfectly stitched forming continuous smooth ML interfaces parallel to the surface of the blazed facets. These layers are analogous to Bragg planes in asymmetrically cut Bragg crystals as schematically shown with dashed lines. Note that the incident light typically does not reach the substrate since a ML stack is chosen thick enough to diffract all the radiation, and the blaze angle of a MBG is entirely defined by the tilt of the layers with respect to the grating surface. The same layer structure can be obtained over very small areas by deposition of a thick multilayer on a flat substrate followed by an oblique slice of the structure, as was previously demonstrated [9].

Calculated diffraction efficiency of a 1st diffraction order of a dense soft x-ray grating versus wavelength is shown in Fig. 1b. The grating had a period of 41.73 nm and a blazed angle of 5.5°, and was coated with a W/B_4C multilayer with d-spacing of 4 nm, composed of 30 pairs of W and B_4C layers of equal thickness. For an incidence angle of 82.75° the Bragg angle is 12.75°. The efficiency curve is shifted with respect to the reflectance curve of the same multilayer at the same Bragg angle towards shorter wavelengths. This is caused by refraction effects which are different for the case of asymmetrical Bragg diffraction as compared to the symmetrical case [10]. The details of refraction effects and their dependence on the asymmetry of diffraction and ML parameters will be reported elsewhere [11].

If the layers of a coating are thicker or thinner than condition (1) requires, the ideal blazing is corrupted. However, our simulations show that diffraction efficiency does not substantially fall and remains high even for a large deviation of the ML d-spacing from the ideal one of 4 nm. This is demonstrated in Fig. 2 where the reflectance of multilayers with different d-spacing is shown with solid lines of different colors, and the efficiency of the respective gratings is shown by lines with solid symbols of respective colors. For example, the reflectance of a ML with D_{ML} = 2.8 nm is 29.6%, while the absolute diffraction efficiency of the MBG coated with this ML is 19% (orange curves and symbols). Therefore, the relative efficiency defined as the ratio of the MBG efficiency to the ML reflectance is 0.64 for h/D_{ML} = 0.7. This is not dramatically lower than the relative efficiency of 0.83 for D_{ML} =4 nm which corresponds to the exact Bragg condition h/D_{ML}=1. The relative efficiency of 0.54 of the MBG with D_{ML} = 5 nm and h/D_{ML}=1.25 emphasizes this point. As we mentioned before, a range of 0.8-1.2 of the h/D_{ML}-ratio is of practical interest for VLS gratings used for typical soft x-ray applications.

Our simulations show that ML-coated VLS gratings with groove density variation of 20% or less can maintain very high efficiency because the blazing condition is rather soft. The drawing in Fig. 3 illustrates the layer structure of such a grating and gives an insight into why the blazing condition is far softer than would otherwise be thought. When the h/D_{ML} ratio deviates from an integer number the ideal stitching of the layers is perturbed and an ideal periodic structure associated with the smooth multilayer interfaces disappears. Instead of the ideal structure composed of smooth layers shown in Fig. 1, a new structure composed of staggered layers forms as shown in Fig. 3. Despite the interface perturbations in the stitching areas, this new structure has a periodicity shown with blue lines. The staggering of the layers can be considered as a sort of interface roughness which is expected to reduce the diffraction efficiency. This is exactly what simulation shows (Fig. 2). The most important thing is that the average slope, ϕ, of the staggered layers is different from the substrate blaze angle, ϕ_0, and can be found as:

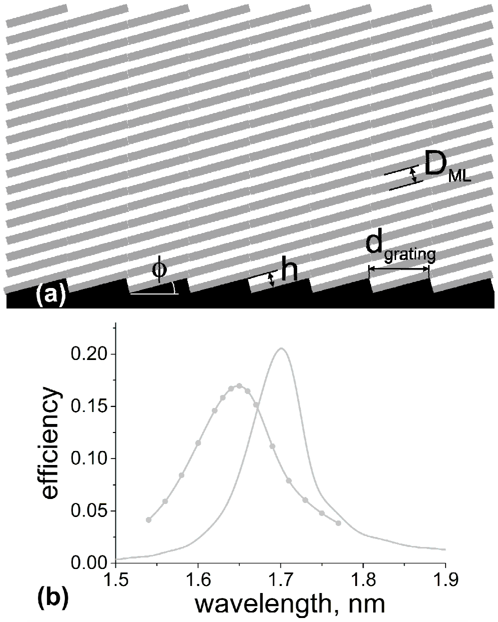

Fig. 1. A MBG with a perfect blazing structure: layers of adjacent grooves form continuous smooth interfaces (a). MBG efficiency (curve with symbols) and ML reflectance (solid curve) versus wavelength (b).

$$tg\phi = \frac{D_{ML}}{d_{grating}}\cos\phi_0 \qquad (2)$$

The staggered layers define a new blaze angle which depends according to formula (2) not only on the substrate blaze angle, but the h/D_{ML} ratio. That means that small errors in groove depth or layer thickness will result in minor changes of the blaze angle with minimal stitching errors and almost no detectable efficiency reduction. This gives a very important practical opportunity to adjust the effective blaze angle of a MBG if necessary. Fabrication of blazed substrates with a precise blaze angle value can be challenging especially for shallow angles. However, the effective blaze angle can be precisely tuned by a proper choice of the layer thickness, which can be easily done by high accuracy deposition techniques.

Since the average slope of the staggered layers varies, the effective Bragg angle changes as well. This results in a change of the resonance wavelength of the staggered multilayer stack and hence in a different shift of the efficiency curve with respect to the reflectance curve for different D_{ML} (Fig. 2).

The amplitude of the stitching errors of the layers of adjacent grooves increases with deviation from the ideal blazing condition. This perturbs constructive Bragg interference and results in reduction of Bragg reflectance and hence loss of diffraction efficiency.

In the example above we considered ultra-dense MBGs with a period of 41.73 nm and a relatively high blaze angle of 5.5°. Use of 1st order gratings where there is mismatch is preferable since the minimal staggering does not harm efficiency. However, fabrication of such dense gratings is challenging from both the substrate fabrication and ML deposition perspectives [12]. A realistic grating should have a longer pitch. We have demonstrated that a MBG with a period of 200 nm can be fabricated with minimal imperfections and an efficiency approaching the theoretical limit [1-3]. For lower groove density gratings one can reduce the blaze angle to keep blazing into the 1st diffraction order or keep the blaze angle high and operate in a high diffraction order. In the latter case however the blazing condition (1) will be much narrower in terms of deviation from the ideal case. For example, the 2nd order grating with a period of 83.46 nm (black curve with open symbols in Fig. 2) has the same efficiency as the 1st order grating with d=41.73 nm for D_{ML}=4 nm (grey curve with solid symbols in Fig. 2). However deviation of the multilayer d-spacing from the optimal one results in efficiency loss which occurs much faster for the less dense grating. The absolute efficiency of the 2nd order grating is as low as 12% for D_{ML}=3.2 nm (shown with a green curve with open symbols in Fig. 2), while the 1st order grating coated with the same multilayer demonstrated efficiency of 22% (green curve with solid symbols). An obvious reason for such efficiency loss is a two-fold increase of the layer staggering as the grating period doubles at the same blaze angle.

The fact the effective slope of staggered layers depends on the h/D_{ML} ratio can be used for VLS MBG gratings. A VLS grating is designed to focus divergent rays coming from a source onto an image plane. Since the angles of incidence and diffraction vary over the grating surface, a certain variation of blaze angle is required to provide the blaze condition for all the area of a blazed VLS grating. It is however extremely difficult to control variation of the blaze angle, and classical diamond ruled grazing incidence gratings have to have a constant blaze angle which provides perfect blazing condition only for a central part of the grating. MBGs offer a unique possibility to provide optimal blazing over a whole clear aperture. Since an effective blazed grating is defined solely by a structure of a ML stack, the local effective blaze angle can be easily controlled by the h/D_{ML} ratio allowing VLS blazed gratings with a variable blaze angle as schematically shown in Fig. 4a.

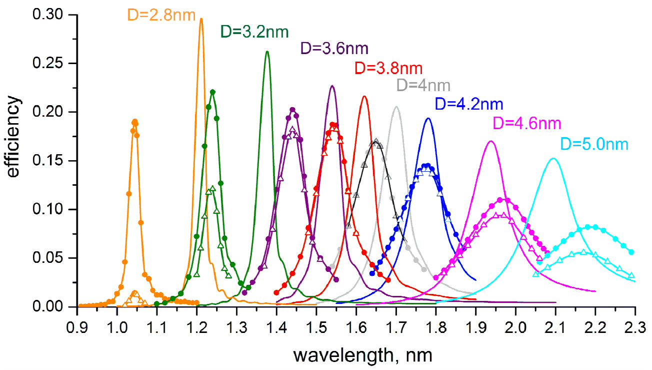

Fig. 2 (color online). Reflectance of W/B4C MLs (solid lines) and diffraction efficiency of MBGs (lines with solid symbols of respective colors) for different ML d-spacing versus wavelength. The substrate parameters, d=41.73 nm and ϕ_0=5.5°, are the same for all the MBGs. Efficiency of 2nd order gratings with d=83.46 nm is shown with lines and open symbols.

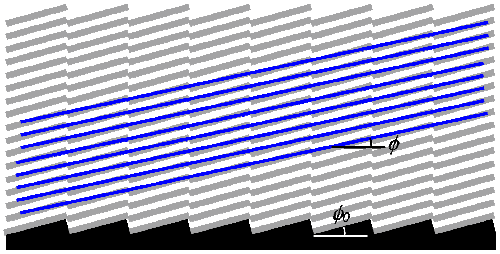

Fig. 3 (color online). A MBG with a deviation from the ideal blazing condition. Staggered layers form a new ML structure with an effective blaze angle, ϕ, different from the substrate blaze angle, ϕ_0.

As an example, we will consider a 100 mm long VLS MBG with the same parameters in the center of the grating (X=0) as the grating shown in Fig. 1: d=41.73 nm, ϕ_0=5.5°, incident angle, α_0 = 82.75°, and coated with the W/B4C multilayer with a constant d-spacing of 4 nm. The source-to-grating and grating-to-image distances were chosen to be of 2 meters each. The diffraction angle, β_0, in the center of the grating is 71.749° for the wavelength of 1.766 nm. Based on simple geometrical considerations and the grating equation, local grating parameters such as the pitch, angles of incidence and diffraction were calculated for each point of the grating. An optimal local blaze angle given by $\phi = (\alpha - \beta)/2$ is shown versus the X coordinate (along the grating length) by a blue line in Fig. 4b.

Since the d-spacing of the multilayer is the same for all the area of the grating, while the grating pitch varies depending on X coordinate, the h/D_{ML} ratio also varies causing variation of the average slope of the staggered layers as schematically shown in Fig. 4b by a red curve. A dashed line in Fig. 4b depicts the substrate blaze angle which is constant. It is seen that the optimal local blaze angle varies significantly along the grating length, and the constant blaze

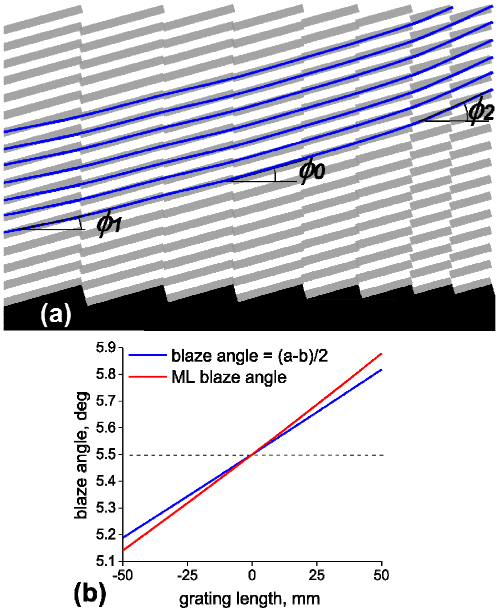

Fig. 4 (color online). Schematic of a VLS multilayer coated grating with a variable blaze angle (a). Variation of the effective blaze angle along the grating length (red line) is close to the optimal local blaze angle (blue line). A dashed line depicts the substrate blaze angle.

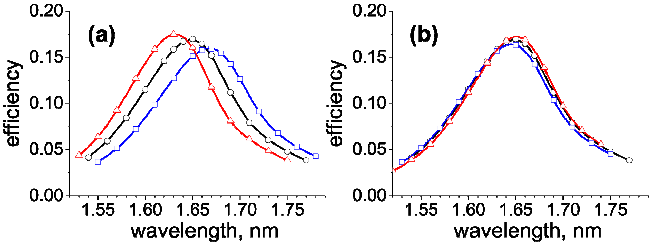

Fig. 5 (color online). (a) Efficiency of a VLS grating coated with a constant d-spacing ML, calculated for three positions with coordinates X= -50 mm (red), X=0 mm (grey), and X= 50 mm (blue) along the grating length. (b) the same as (a), but for a laterally graded ML.

angle cannot provide the true blazed condition for all parts of the grating. At the same time the effective blaze angle formed by the staggered multilayer stack (blue line in Fig. 4b) is quite close to the optimal one, so strong blazing and hence high diffraction efficiency can be expected for the whole area of the VLS MBG. To verify this, we simulated the efficiency of different parts of the VLS MBG by calculation of the efficiency of three different constant groove density MBGs. Periods of the gratings and geometry of the diffraction correspond to the parameters of the VLS MBG grating considered above at the coordinates X = -50 mm, X = 0 mm, and X = 50 mm. The bandwidth (i.e. a dependence of the efficiency on wavelength) for all three gratings is shown in Fig. 5a.

The mismatch of the efficiency curves in Fig. 5a is mostly caused by deviation of the effective blaze angle obtained from the constant d-spacing ML on the VLS saw-tooth substrate from the ideal one (Fig. 4b). A longitudinally graded ML can be used for precise tuning of the local blaze angle to its optimal value (blue line in Fig. 4b) and matching the efficiency curves for different parts of the VLS MBG. For example, if the ML d-spacing D_{ML}= 4.037 nm at the coordinate X=-50 mm, and D_{ML}= 3.959 nm for X= 50 mm, the respective bandwidth curves match very well the one for the central grating area (X=0) with D_{ML}=4 nm as shown in Fig. 5b. The residual marginal mismatch is caused by slight changes of the effective d-spacing for the staggered layers, and also can be corrected by further d-spacing optimization.

In summary, we found that the blazing condition is quite relaxed for dense MBGs. The diffraction efficiency reduces slowly with a deviation from the ideal blazing condition (1). The deviation results in a staggered layer structure of the multilayer stack giving an effectively modified blaze angle different from the blaze angle of a saw-tooth substrate. This gives a unique opportunity to precisely tune the effective blaze angle with a proper choice of the ML d-spacing. Deposition of a ML on a VLS substrate results in a ML stack with variable effective blaze angle. The local blaze angle variation can be made very close to the ideal one. A graded multilayer can provide perfect blazing for the whole area of a VLS MBG. This defines a new class of x-ray gratings in which near perfect blazing can be had for variable line space gratings.

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